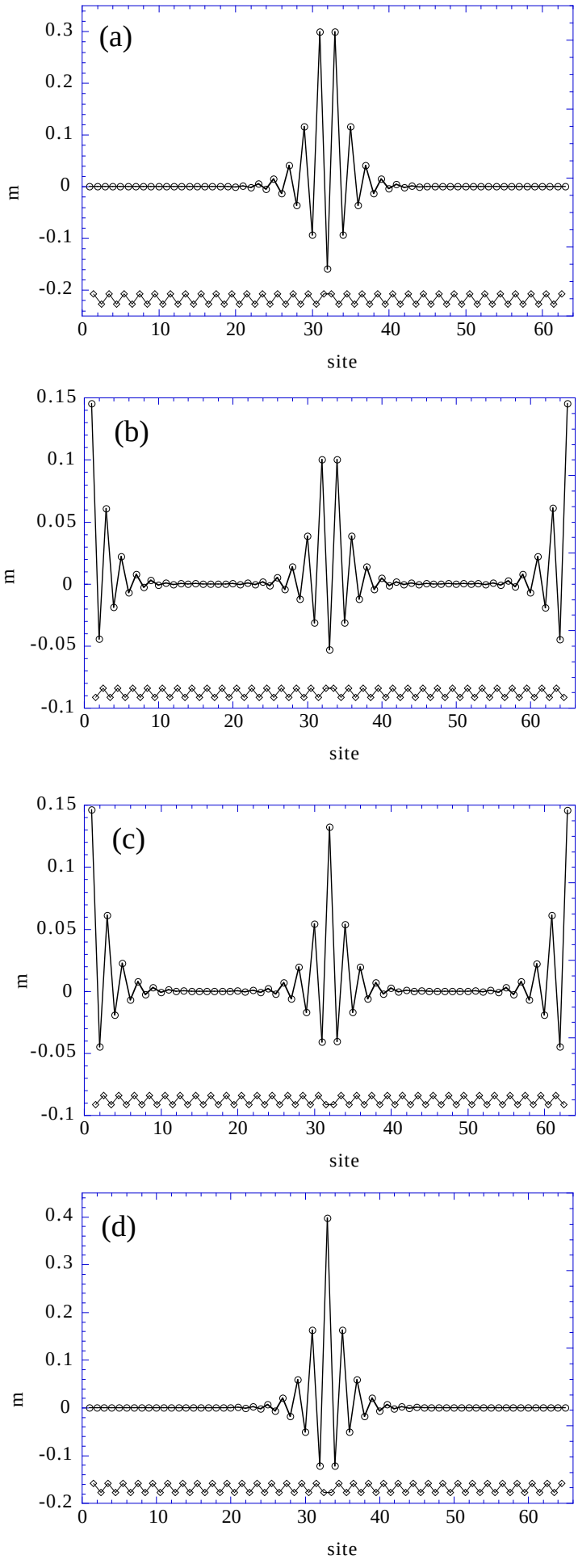


Fig. 1 M. Nishino, et al.

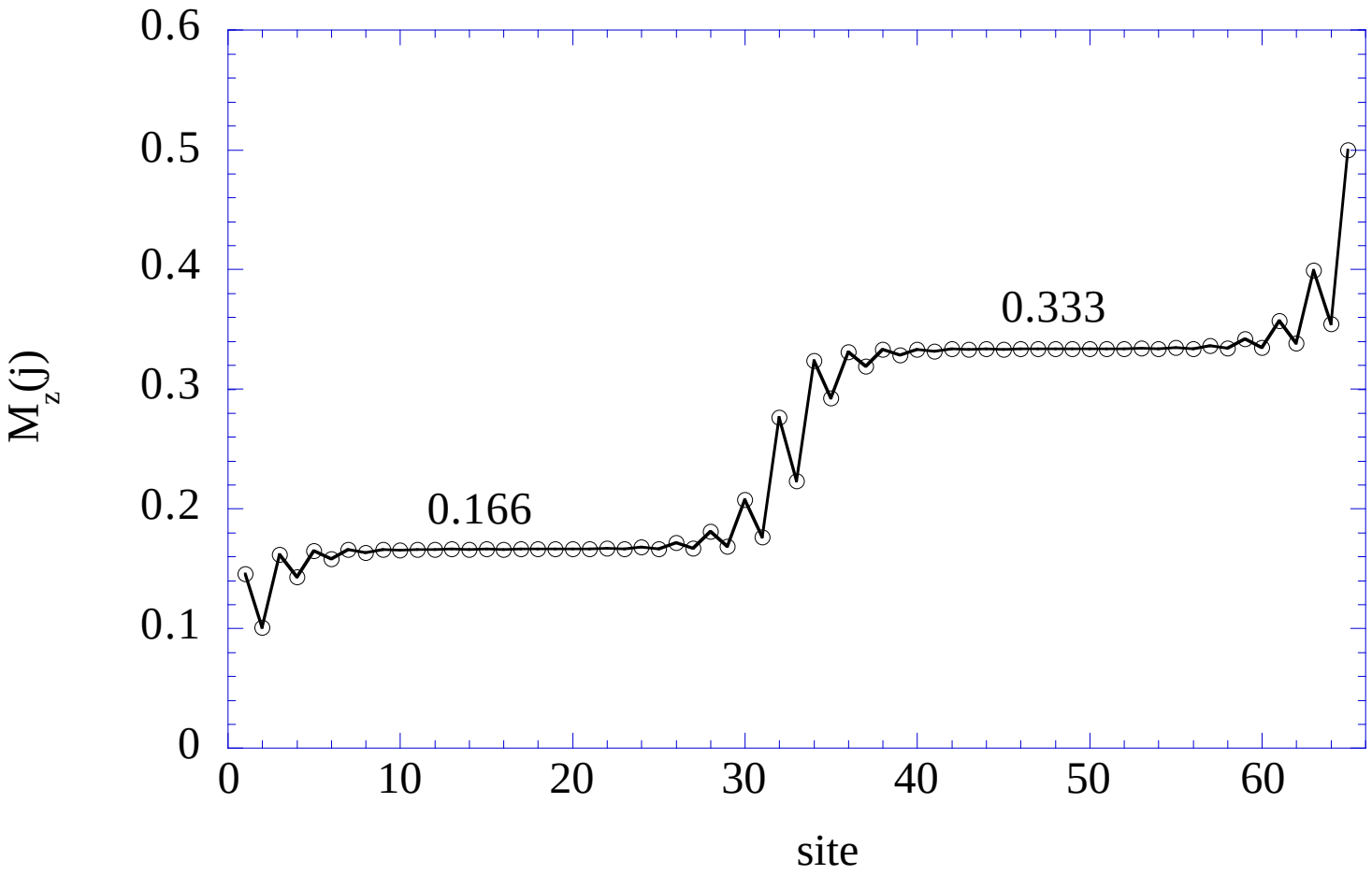
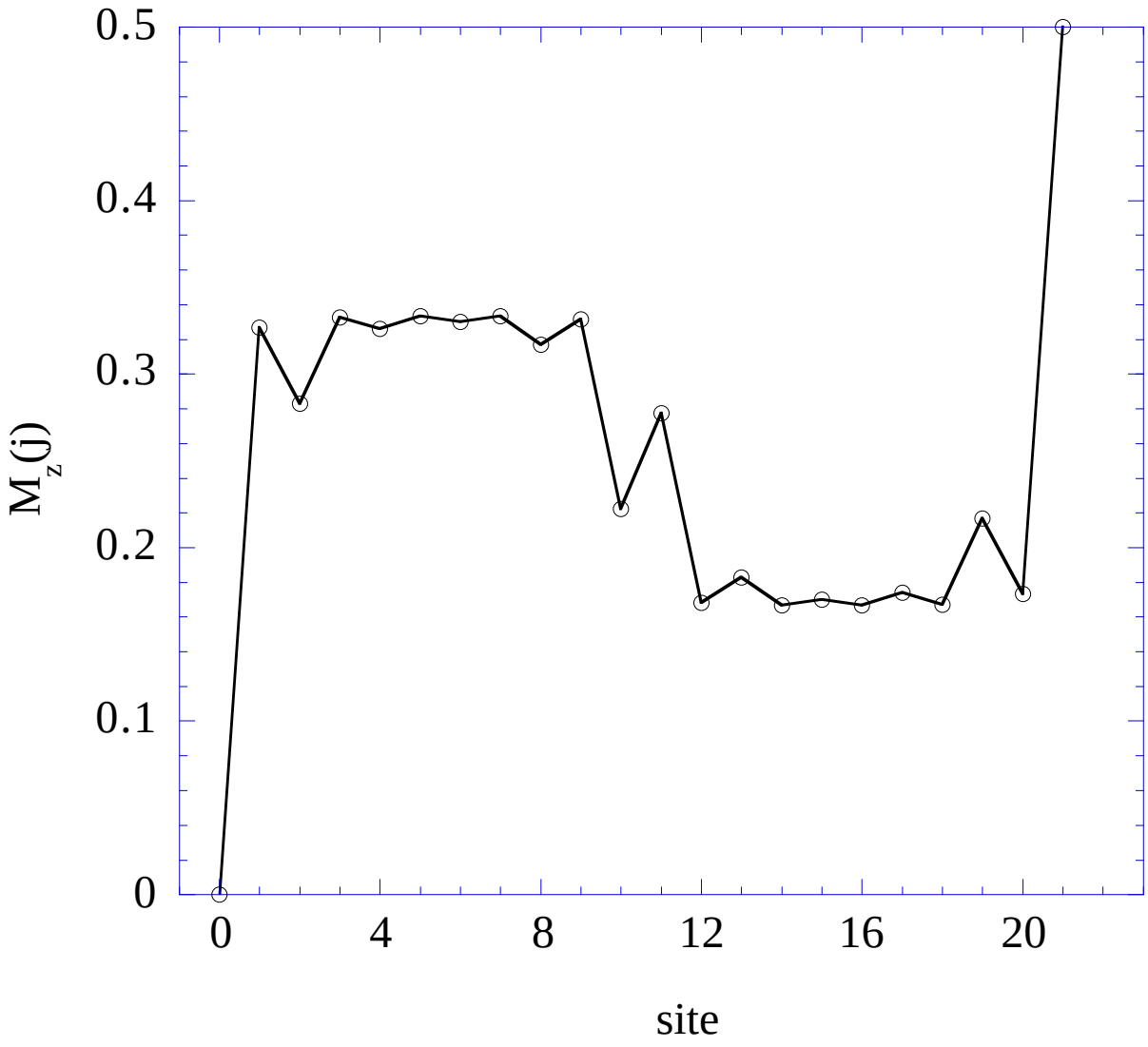


Fig. 2 M. Nishino, et al.



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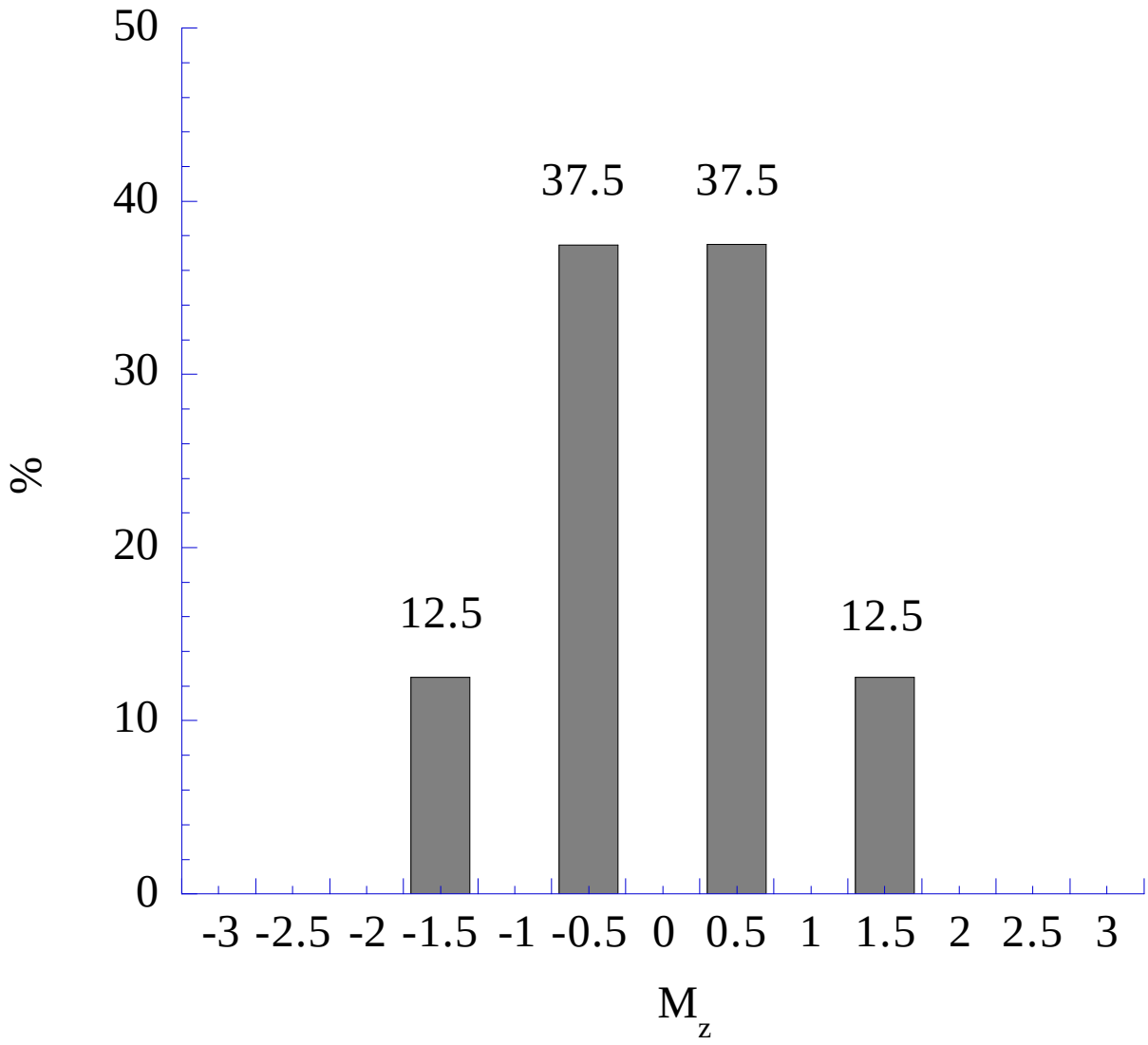

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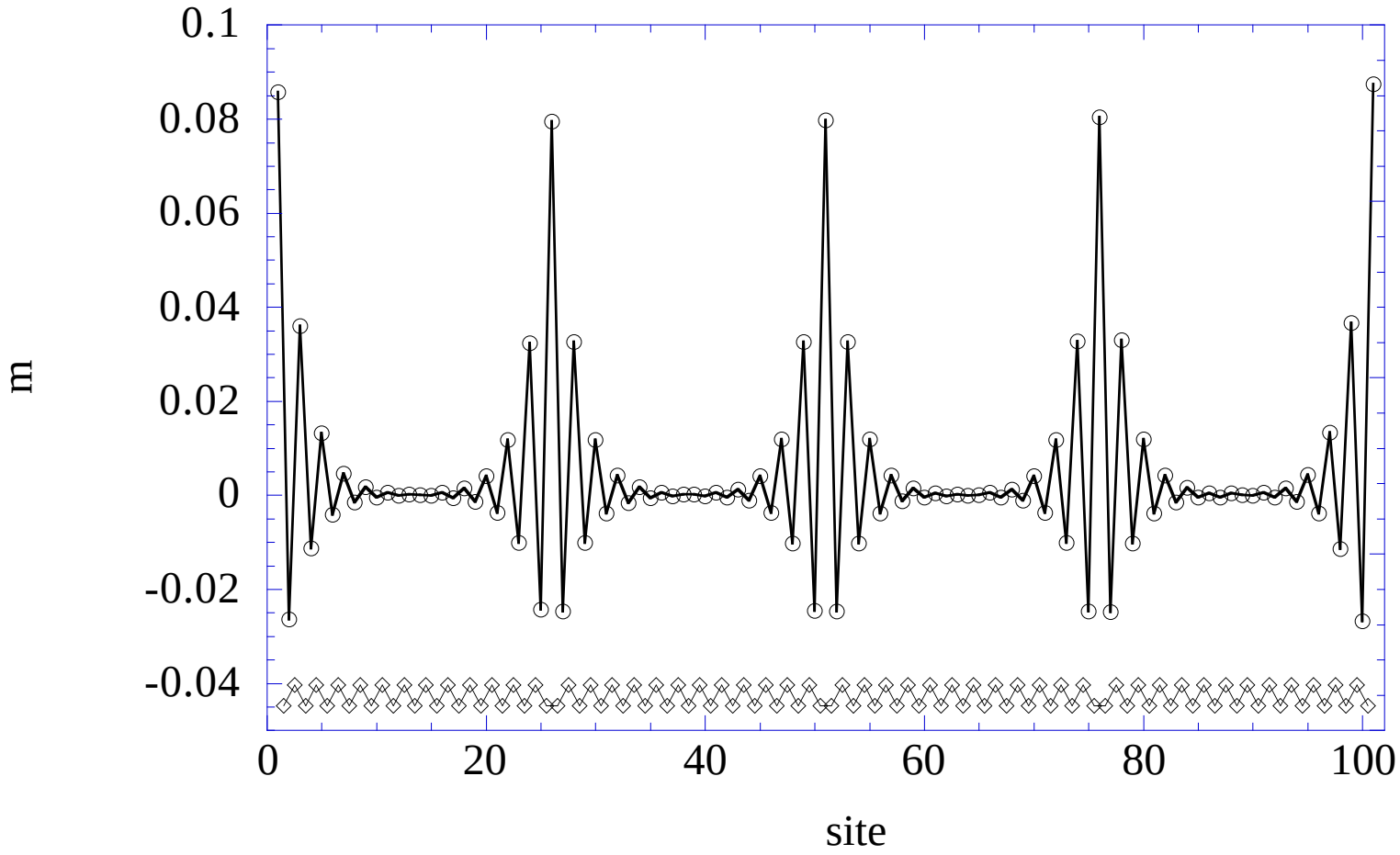

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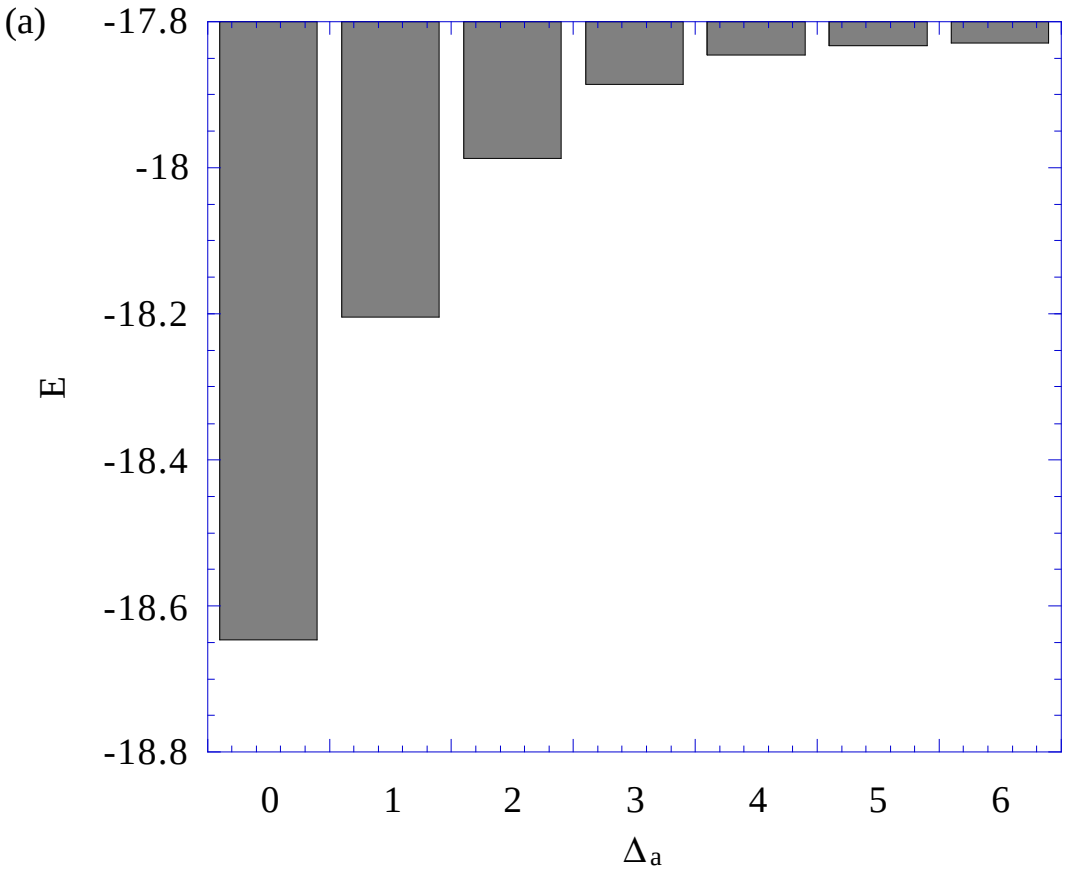

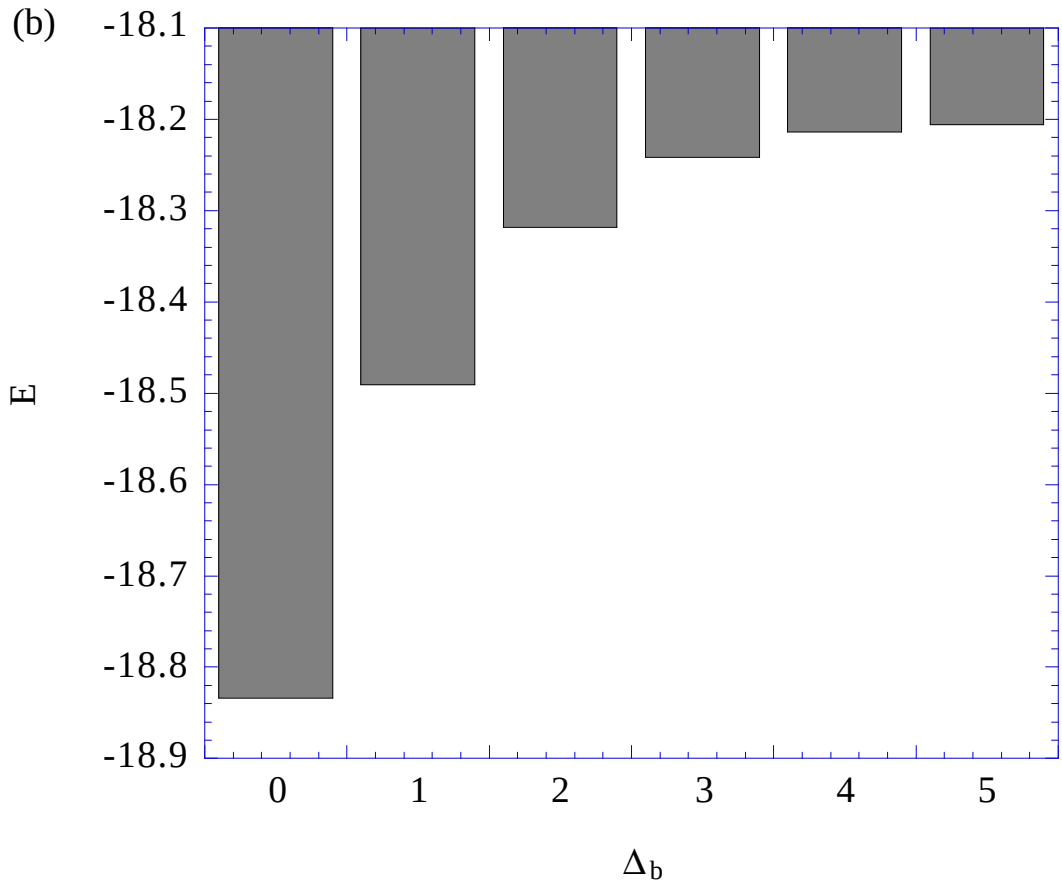

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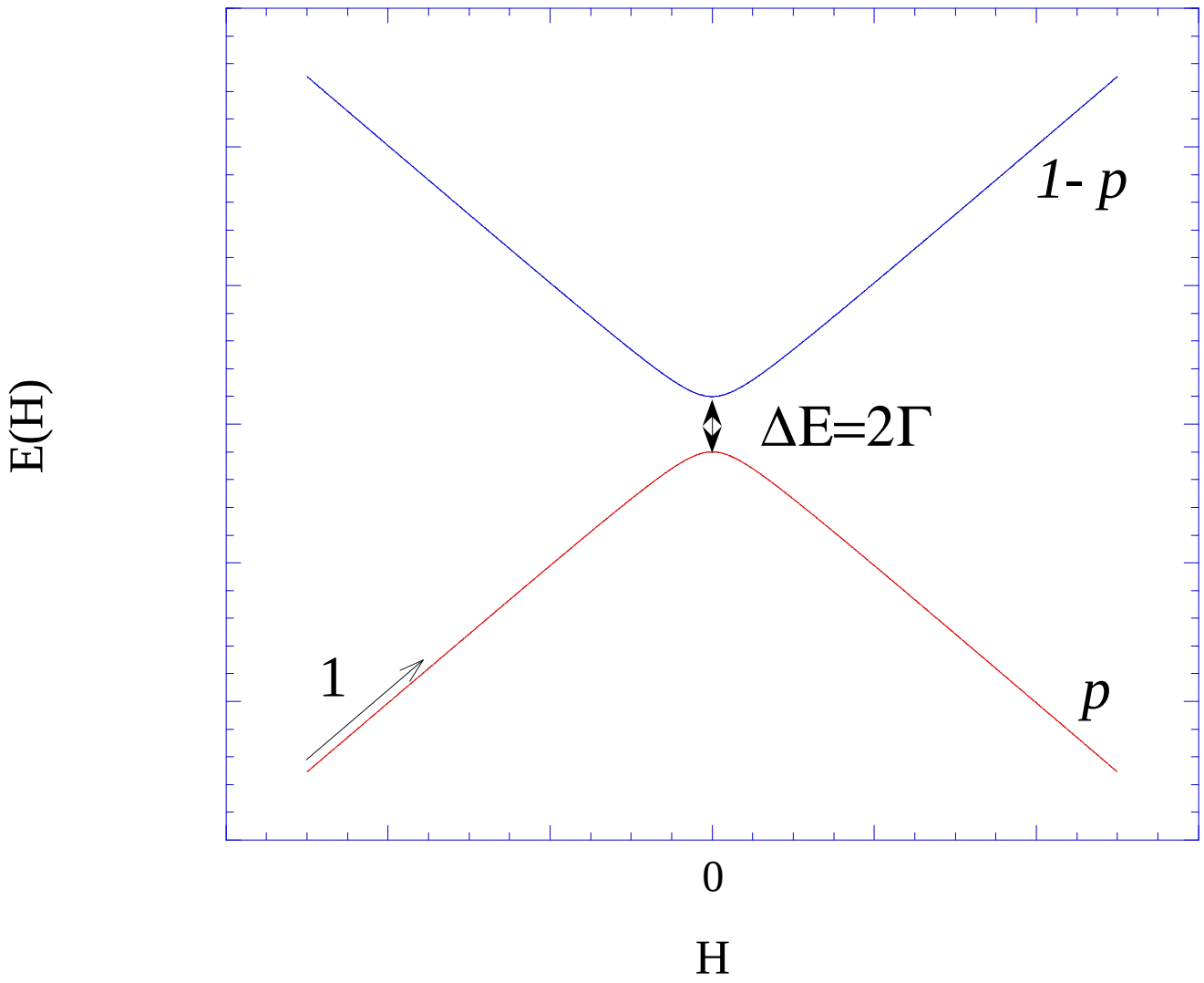

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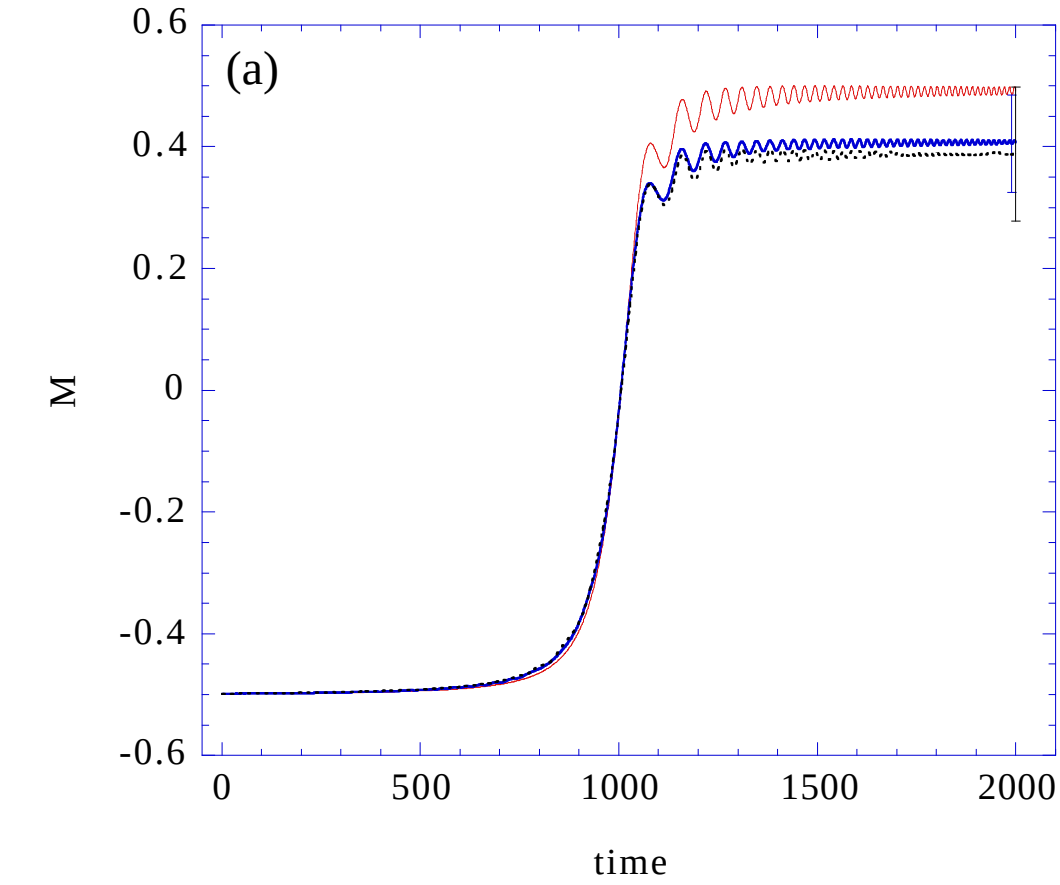

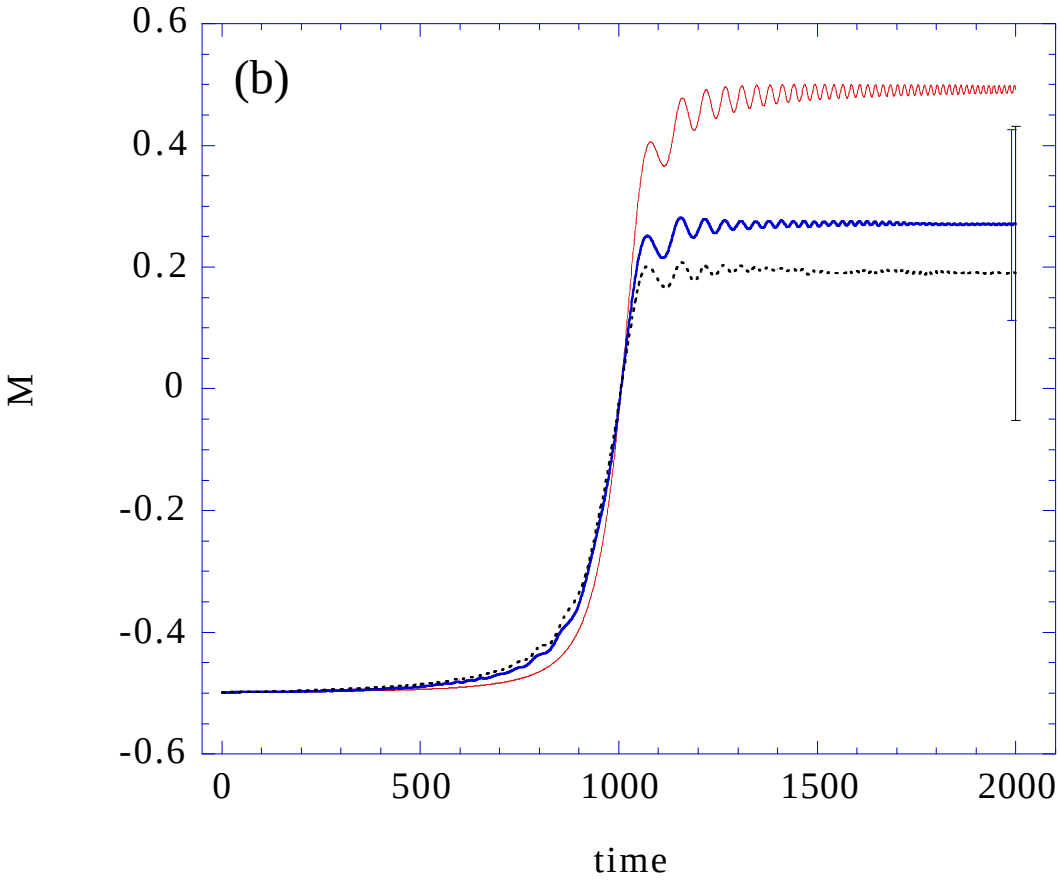

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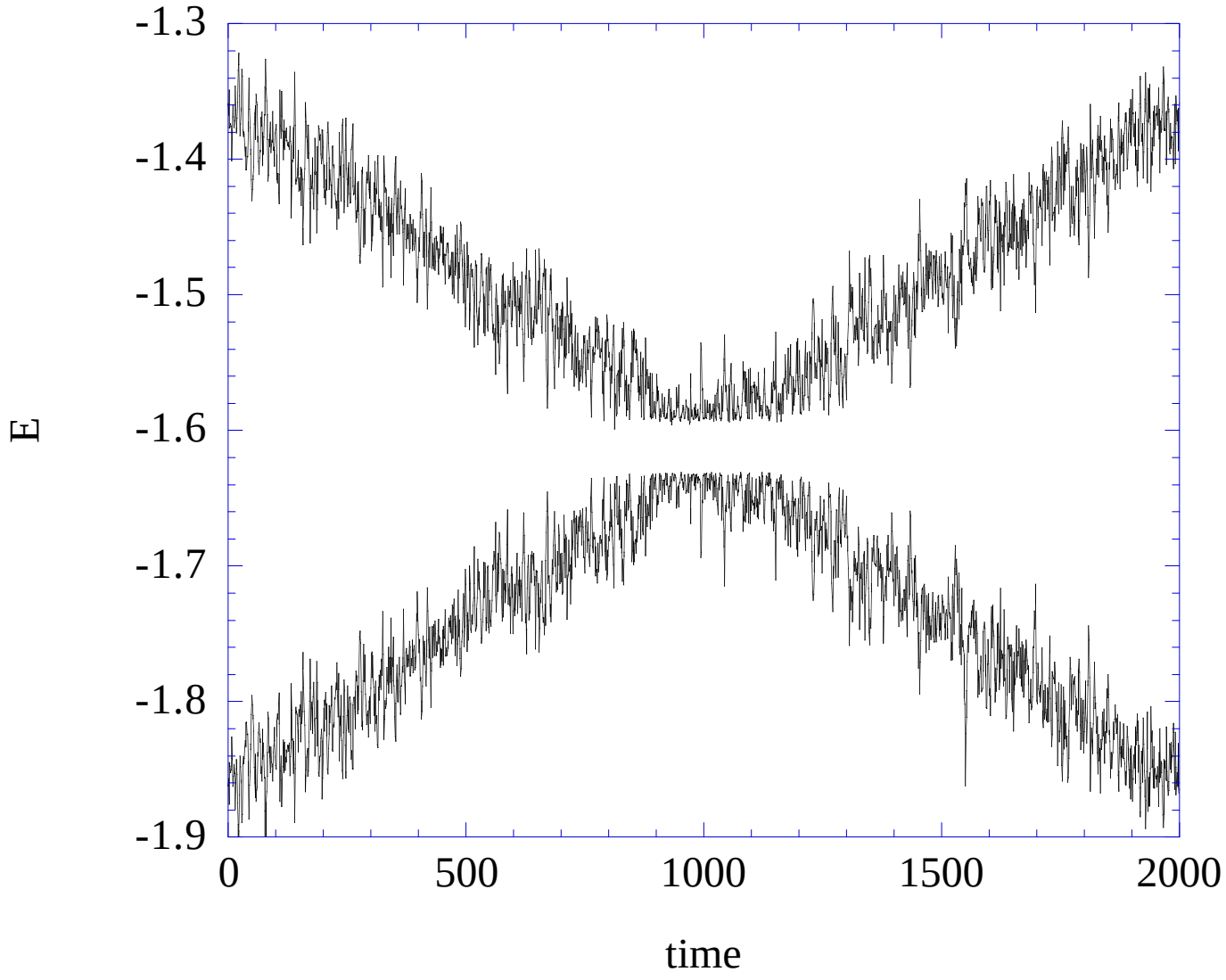

Fig. 9 M. Nishino, et al.

Local magnetic structures induced by inhomogeneities of the lattice in $S = 1/2$ bond-alternating chains and response to time-dependent magnetic field with a random noise

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We study effect of inhomogeneities of the lattice in the $S = 1/2$ bond-alternating chain by using a quantum Monte Carlo method and an exact diagonalization method. We adopt a defect in the alternating order as the inhomogeneity and we call it ''bond impurity''. Local magnetic structures induced by the bond impurities are investigated both in the ground state and at very low temperatures. The local magnetic structure can be looked on as an effective $S = 1/2$ spin and the weakness of the interaction between the local structures causes the quasi-degenerate states in the low energy. We also investigate the force acting between bond impurities and find that the force is generally attractive. We also study the dynamical property of the local magnetic structure. While the local magnetic structure behaves as an isolated $S = 1/2$ spin in the response to a time-dependent uniform field, it is found to be robust against the effect of a random noise applied at each site individually in the sweeping filed.

I. INTRODUCTION

In the low dimensional quantum spin systems, it has been turned out that the quantum mechanical effect, in particular the mechanism of the singlet pair formation, plays an important role for the ground state spin configuration [1–3]. There have been found a wide variety of peculiar arrangements of the singlet pairs in the ground state which brings new types of singlet (or nonmagnetic) ground state phases such as VBS [3], RVB [4,5], etc. As general characteristics of these systems, a finite energy gap exists between the ground state and excitation states and the correlation length in the ground state is finite. If a lattice has some inhomogeneities such as impurity sites, defects of periodicity, and edge points, etc., then local magnetic structures are induced around them [6–9]. Property of such induced moments is one of the most interesting current topics.

In this paper we will study the interaction between the induced moments and also dynamical properties of such moments in the bond-alternating Heisenberg antiferromagnetic (HAF) chain. This model is one of the simplest systems of the singlet ground state which consists of singlet states at strong bonds. The magnetic susceptibility and specific-heat of this model was studied in detail as a function of the ratio of the alternation coupling constants by Duffy and Barr [10]. Various materials corresponding to this model have been studied experimentally, i.e., aromatic free-radical compounds [11], $Cu(NO_3)_2{\cdot}2.5H_2O$ [12], and $(VO)_2P_2O_7$ [13], etc. The ratio of the alternation coupling constants for theses materials has been estimated comparing with the theoretical results [11]. This system has been also extensively studied concerning with the spin-Peirels transitions [14–16].

Here we consider a defect of the alternating order of the bonds, such as $\cdots$ABAB$\underline{\text{AA}}$BAB$\cdots$ or $\cdots$ABA$\underline{\text{BB}}$ABAB$\cdots$, where A or B denotes the strength of bonds (the magnitude of exchange constant). At this defect the singlet dimer state cannot be formed there. First we study how a magnetic structure appears at these positions. In this paper we call such a defect of the alternating order ''bond impurity''. Furthermore, the induced magnetic structure depends on whether the edge bond is A or B. Bond impurity effects in the uniform HAF have been investigated in our previous paper [17] and we compare the role of the bond impurity in the present model with them.

Next, we focus on what kind of interactions act between these locally induced magnetic structures. We study the force by investigating the dependence of the

ground state energy on the distance between the impurities for various types of configurations of defects. The force between the bond impurities has been also studied for the uniform HAF [17]. There we found that the attractive force acts. In the present model we again find only attractive force regardless of the types of configuration.

Due to the finite correlation length of the present model, the induced moments behave almost independently. Thus we can regard such a local moment as a microscopic moment. Because recently the technology in microscopic processing makes remarkable progress and the analyses in microscale or nanoscale phenomena have become possible, the quantum phenomena in microscale or nanoscale have received much attention. For example, the resonant tunneling phenomena have been observed in recent experiments on high-spin molecules (Mn_{12}) [18–20] and the concept of quantum tunneling of the magnetization (QTM) has become a topic of interest. Recently the adiabatic motion of spin 1/2 was observed in V_{15} and the effects of thermal disturbance on the dynamics has been discussed [21]. We have studied the tunneling dynamics from viewpoint of the nonadiabatic transition [22–25].

Under a time-dependent magnetic field, how does that local magnetic structure behaveH We study the response of the magnetization to a sweeping magnetic field. Although the induced moment consists of several spins, the total magnetization behaves as a single spin when a uniform field is applied. Under a sweeping magnetic field the behavior of magnetization is described by the Landau-Zener-Stückelberg (LZS) formula [26–28]. In realistic situations, noise disturbs the simple behavior of LZS formula [29,30]. Furthermore, if the noise acts independently at each site, the behavior of induced moment (a cluster of spins) is expected to be different from that of isolated single spin. We investigate effects of such individual noise at each site on the dynamical properties.

This paper is organized as follows. In the next section, we explain briefly the method used in this study. In Sect. III, effects of bond impurities on the magnetic structure in bond-alternating chains are studied. In Sect. IV, we study the force between bond impurities. In Sect. V, we investigate the response of the magnetization to a sweeping field. Sect. VI is devoted to the summary and discussion.

II. MODEL AND METHOD

The Hamiltonian treated in the present paper is given by

$$\mathcal{H} = \sum_i J_{i,i+1} \mathbf{S}_i \cdot \mathbf{S}_{i+1}, \tag{1}$$

where $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$ are the $S = 1/2$ spin operators at the site i. We study the bond-alternating chain where $J_{i,i+1}$ changes alternately among J_1 (a strong bond) and J_2 (a weak bond). Here we consider defects of the alternation which cause inhomogeneities of the lattice (bond impurities). To study low temperature properties of the model, we mainly use the loop algorithm of the continuous time quantum Monte Carlo method (LCQMC) [31,32] with a method of specification of the magnetization M_z [7,17]. This method overcomes the problem of long autocorrelation in Monte Carlo update and allows us to study systems at very low temperatures. In the present work, we performed 10^5 Monte Carlo steps (MCS) for getting equilibrium of the system and 10^6 MCS to obtain quantities in the equilibrium state. Here a MCS means an update of the whole spins.

In order to study the dynamical response of spins under a time-dependent external field, we investigate the following system:

$$\mathcal{H} = \sum_i J_{i,i+1} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + 2\Gamma \sum_i S_i^x - \sum_i (H(t) + h_i(t)) S_i^z, \tag{2}$$

where $H(t)$ is a time-dependent external field and $h_i(t)$ is a random noise applied to each site individually. Γ is the transverse field which represents terms for quantum fluctuation of M_z. The time evolution of the state is obtained by the time-dependent Schrödinger equation (TDSE)

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \mathcal{H} |\Psi(t)\rangle, \tag{3}$$

where $|\Psi(t)\rangle$ denotes the wave function of the spin system at time t. We set $\hbar = 1$. Equation (3) is solved using the fourth-order fractal decomposition [33],

$$e^{-it\mathcal{H}} = [S_2(-itp_2)]^2 S_2(-it(1-4p_2))[S_2(-itp_2)]^2, \tag{4}$$

where $S_2(x) = e^{x\mathcal{H}_1/2} e^{x\mathcal{H}_2} e^{x\mathcal{H}_1/2}$ with $p_2 = (4 - 4^{\frac{1}{3}})^{-1}$, putting

$$\mathcal{H}_1 = \sum_i J_{i,i+1} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + 2\Gamma \sum_i S_i^x,$$
$$\mathcal{H}_2 = -\sum_i (H(t) + h_i(t)) S_i^z.$$

As the initial state, we set the applied field to its minimum value $H(t=0) = -H_0 < 0$, and put the system to be the ground state for this field. Then we sweep the filed as

$$H(t) = -H_0 + ct. \tag{5}$$

Beside this sweeping field, we provide a random noise with an exponential-decaying autocorrelation function $\{h_i(t)\}$ by a Langevin equation (Ornstein-Ulenbeck process),

$$\dot{h}(t) = -\gamma h(t) + \eta(t). \tag{6}$$

Here $\eta(t)$ is a white gaussian noise,

$$\langle \eta(t) \rangle = 0 \quad \text{and} \quad \langle \eta(0)\eta(t) \rangle = A^2 \delta(t), \tag{7}$$

where A is amplitude, γ is damping factor. Thus obtained random process $h(t)$ has the properties

$$\langle h(t) \rangle = 0 \quad \text{and} \quad \langle h(0)h(t) \rangle = \frac{A^2}{2\gamma} \exp(-\frac{t}{\tau}), \tag{8}$$

where $\tau = 1/\gamma$. The dynamics of magnetization is obtained as

$$M(t) = \langle \Psi(t) | \sum_i S_i^z | \Psi(t) \rangle. \tag{9}$$

If the magnetic field changes rather slowly, i.e., the sweep rate is rather small, $|\Psi(t)\rangle$ changes adiabatically. In this case the state stays in the ground state of the system for the current field $H(t)$, and the magnetization follows the value of the ground state. When the sweeping rate becomes large the system cannot follow the change of the field completely, and the nonadiabatic transition occurs. The probability to stay in the ground state was given by LZS formula as

$$p = 1 - \exp(\frac{-2\pi\Gamma^2}{c}). \tag{10}$$

When the effect of noise does not become negligible, the noise disturbs the quantum process and this probability changes [29].

III. BOND IMPURITY IN BOND-ALTERNATING CHAINS

We investigate magnetic structures in the system (1) with a bond alternation $\cdots J_1 J_2 J_1 J_2 \cdots$, where $J_1 > J_2$. We study effects of a defect in the alternation, such as $\cdots J_1 J_2 J_1 J_2 \underline{J_1 J_1} J_2 J_1 J_2 J_1 \cdots$. Beside this defect, magnetic structures can be induced at the edges as naturally understood from the VBS picture, i.e., an unpaired spin causes an induced magnetization (see the figures). Thus we study the following four systems of the bond configurations:
(a) a chain of 63 sites where the two strong bonds are at the center and both edges terminate with a strong bond, $(J_1 J_2 \cdots J_1 J_2 \underline{J_1 J_1} J_2 J_1 \cdots J_2 J_1)$
(b) a chain of 65 sites where the two strong bonds are at the center and both edges terminate with a weak bond, $(J_2 J_1 \cdots J_1 J_2 \underline{J_1 J_1} J_2 J_1 \cdots J_1 J_2)$
(c) a chain of 63 sites where the two weak bonds are at the center and both edges terminate with a weak bond, $(J_2 J_1 \cdots J_2 J_1 \underline{J_2 J_2} J_1 J_2 \cdots J_1 J_2)$
and
(d) a chain of 65 sites where the two weak bonds are at the center and the edges terminate with a strong bond $(J_1 J_2 \cdots J_2 J_1 \underline{J_2 J_2} J_1 J_2 \cdots J_2 J_1)$.

Here we take the strong bond to be $J_1 = 1.3$ and the weak bond to be $J_2 = 0.7$. For this set of bonds, the correlation length is estimated as $\xi \simeq 0.82$ (see Appendix). Here we take $k_{\rm B}$ as a unit of energy ($k_{\rm B} = 1$). These four models have odd number of spins and their ground state is doublet according to the Lieb-Mattis theorem [34]. We performed simulations at $T = 0.01$ in the $M_z = 1/2$ space to study magnetic structures in the low energy state. The magnetization profiles $\{m_i\}$ of (a)-(d) are drawn in Fig. 1, where $m_i = \langle S_i^z \rangle$ and $\langle\ \rangle$ denotes the canonical average at a given temperature. A magnetization is induced locally around the impurity. First we consider the cases where the bonds at edges are strong, i.e., the model (a) and (d). If we allocate a singlet pair at each strong bond, neighboring two strong bonds remain at the center in the model (a), while one site remains in the model (d). The magnetization of $M_z = 1/2$ is assigned in the remaining part at the center of the lattices to induce a local magnetic structure. Because the edge bonds are strong, no magnetization is induced at the edges. Figures 1(a) and (d) are considered to describe well the magnetization profiles of the ground state since these are gapful systems without quasi-degenerate states within a subspace with a fixed magnetization (i.e., $M_z = 1/2$). We find that M_z is distributed only into the $\pm 1/2$ space in the simulations at this temperature.

In the models (b) and (c), when we allocate singlet state at the strong bond, there are three positions for magnetic moments, i.e., the center and both edges. Indeed in the both models (b) and (c), magnetizations are induced around the impurity and both edges as shown in Fig. 1. In order to study the distribution of magnetization in the lattice, we introduce the summation of the magnetization per site from the left edge site

$$\mathcal{M}_z(j) = \sum_{i=1}^{j} m_i. \tag{11}$$

We show this quantity for the model (b) in Fig. 2. There the values of the left plateau and right plateau are 0.166 and 0.333, respectively. From this figure we find a spin 1/6 locates at each local structure. This deceptive fractional magnetization is considered to come from mixing of states.

Looking on the local magnetic structure as an effective $S = 1/2$ spin interacting by an effective exchange $\tilde{J}$, this system is modeled by a three-site Heisenberg model $\mathcal{H} = \tilde{J}\mathbf{S}_1 \cdot \mathbf{S}_2 + \tilde{J}\mathbf{S}_2 \cdot \mathbf{S}_3$. In the $M_z = 1/2$ space the eigenvalues are

$$E_1 = -\tilde{J}, E_2 = 0, \text{ and } E_3 = \tilde{J}/2. \tag{12}$$

The corresponding eigenvectors are denoted by $|\phi_i\rangle, (i = 1, 2, \text{and} 3)$. The expectation values of magnetization of spins in each state are

$$\begin{aligned} &\langle \phi_1 | S_1^z | \phi_1 \rangle = \langle \phi_1 | S_3^z | \phi_1 \rangle = 1/3 \ \text{ and } \ \langle \phi_1 | S_2^z | \phi_1 \rangle = -1/6, \\ &\langle \phi_2 | S_1^z | \phi_2 \rangle = \langle \phi_2 | S_3^z | \phi_2 \rangle = 0 \quad \text{ and } \ \langle \phi_2 | S_2^z | \phi_2 \rangle = 1/2, \\ &\langle \phi_3 | S_1^z | \phi_3 \rangle = \langle \phi_3 | S_2^z | \phi_3 \rangle = \langle \phi_3 | S_3^z | \phi_3 \rangle = 1/6. \end{aligned} \tag{13}$$

In the gapped spin system the correlation function decays exponentially and the effective coupling between the induced moments is expected to be very small [7,8], i.e., $\tilde{J} \ll 1$. Thus these states are considered to be almost degenerate even at this temperature ($T = 0.01$), although there are energy gaps of order $O(\tilde{J})$ between the state $|\phi_1\rangle$, $|\phi_2\rangle$, and $|\phi_3\rangle$. In such a case the three states appear in the equal probability, and the expectation value of magnetization is given by an equal-weight average in the three state. That is, $\langle S_1^z\rangle$, $\langle S_2^z\rangle$, and $\langle S_3^z\rangle$ are given by $(1/3+0+1/6)/3 = 1/6$, $(-1/6+1/2+1/6)/3 = 1/6$, and $(1/3+0+1/6)/3 = 1/6$, respectively. These values correspond to the observed deceptive fractional magnetization.

In order to confirm the above modeling we perform the following two investigations. First, we investigate a short chain of $L = 21$ by an exact diagonalization method in order to check that the ground state of the type (b) is represented by $|\phi_1\rangle$ of the three-spin model. Here we choose a chain of a shorter correlation length because the length of the chain is short. Namely, we set $J_1 = 2$ and $J_2 = 0.5$, where $\xi \ll 1$. Fig. 3 shows the summation of the magnetization from the left edge site (Eq. (11)) for this model. The local magnetization around the left edge is about 1/3 which corresponds to $\langle\phi_1|S_1^z|\phi_1\rangle$. This causes the left plateau. The local magnetization around the impurity at the center is about $-1/6$ ($\langle\phi_1|S_2^z|\phi_1\rangle$). Therefore the right plateau is 1/6 ($\langle\phi_1|S_1^z|\phi_1\rangle + \langle\phi_1|S_2^z|\phi_1\rangle$). Finally adding the local magnetization around the right edge (1/3), $\mathcal{M}_z(21)$ terminates at 1/2. Thus the ground state $|\phi_1\rangle$ represents well that of the type (b) model.

Second, to confirm the quasi-degeneracy in the model (b), we check the distribution of M_z in the Monte Carlo simulation, which is shown in Fig. 4. Here the distribution for $M_z = 3/2$ is about 12.5 %. Because there are three states in the $M_z = 1/2$ space and one state in the $M_z = 3/2$ space in the three-spin model, this distribution indicates that these four states are equally populated and that $T = 0.01$ is much higher than the energy gaps between these four states. In the three-spin model the eigenvalue of the state of $M_z = 3/2$ is $\tilde{J}/2$, while the eigenvalues of the state of $M_z = 1/2$ are $-\tilde{J}$, 0, and $\tilde{J}/2$ (Eq. (12)). In the $M_z = 3/2$ space we observe $S = 1/2$ moment at each local structure which represents the state $|+++\rangle$ in the effective three-site model. The values $\{m_i\}$ are almost three times as large as those of Fig. 1 (b). In principle we can obtain the energy gap from the temperature dependence of the distribution [7]. However it is too small to detect here.

We find a similar scenario for the model (c). Thus we conclude that in bond-alternating systems, local magnetic structures are induced by a bond impurity or weak edge bonds as an effective $S = 1/2$ spin and they behave almost independently.

Now let us examine more detailed structures of the local magnetic structures. In the case (a) a negative magnetization appears at the middle site, while in the case (d) a positive magnetization appears there. The interaction of the three spins at the center of the model (a) is approximately represented by the three-spin model with the strong bonds. Here the magnetizations at the center of the model (a) are distributed as about (1/3, −1/6,1/3). On the other hand in the model (d) a spin at the center is isolated from the others.

The local magnetic structures in the present model are well isolated. Therefore we can locate such magnetic structures as we desire. In Fig. 5 we show a magnetization profile which has five positions of induced structures in a chain of $L = 101$. This system has three J_2J_2 defects and weak edge bonds. This configuration is obtained at a very low temperature ($T = 0.01$) in the space of the total magnetization $M_z = 1/2$. Each moment almost behaves independently. Thus magnetization at each location is given by an average over all the possible states. In the present case, each local moment has a deceptive magnetization 1/10. Furthermore we confirmed that the distribution of magnetization $P(M_z)$ is given by a binomial distribution

$$P(M_z) = \frac{1}{2^5}\frac{5\,!}{(5-2|M_z|)\,!\,(2|M_z|)\,!}. \tag{14}$$

IV. FORCE BETWEEN TWO DEFECTS IN AN ALTERNATING CHAIN

When a bond-alternating system has impurities, what kind of interaction does exist between them, attractive or repulsive? We study the force between the bond impurities in this section. We estimate the ground state energies of the spin system in various fixed configurations of bonds and compare the ground state energies as a function of the distance between the bond impurities.

In the alternating chain ($\cdots J_1J_2J_1J_2\cdots$), the system may have a pair of defects by shifting a position of a strong bond by one.

$$\cdots J_1J_2\underline{J_1J_1}\underline{J_2J_2}J_1J_2\cdots. \tag{15}$$

If we shift the position furthermore, the system has a configuration

$$\cdots \underline{J_1J_1}J_2J_1\underline{J_2J_2}\cdots, \tag{16}$$

etc. We study dependence of the energy on the distance (Δ_a) between the positions of J_1J_1 and J_2J_2. We define $\Delta_a = 0$ for the case of no defect, $\Delta_a = 1$ for the configuration (15), $\Delta_a = 2$ for the configuration (16) and so on. In Fig. 6 (a) we plot the ground state energy as a function of Δ_a obtained by an exact diagonalization for $L = 24$ with $J_1 = 2$ and $J_2 = 1$ in the periodic boundary condition (PBC). The ground state energy becomes larger as Δ_a becomes larger. Therefore we find an attractive force between the impurities (J_1J_1 and J_2J_2).

Next another situation is considered. If one J_2 is exchanged by J_1 in the alternating chain, the system has a configuration

$$\cdots J_1 J_2 \underline{J_1 J_1 J_1} J_2 J_1 \cdots . \tag{17}$$

We define $\Delta_b = 0$ for this configuration.Shifting a position of a J_1 by one, the system has two $J_1 J_1$ pairs and has a configuration,

$$\cdots \underline{J_1 J_1} J_2 \underline{J_1 J_1} \cdots . \tag{18}$$

We define this distance between $J_1 J_1$ and $J_1 J_1$ as $\Delta_b = 1$. Furthermore, $\Delta_b = 2$ is defined for the configuration (19) and etc.

$$\cdots \underline{J_1 J_1} J_2 J_1 J_2 \underline{J_1 J_1} \cdots . \tag{19}$$

The ground state energies for a PBC chain of $L = 24$ are shown as a function of Δ_b in Fig. 6 (b). We also study the interaction between $J_2 J_2$ and $J_2 J_2$, where we define the distance between the impurities in the same way. We again found that the ground state energy increases as the distance becomes larger. Thus it has been found that an attractive force acts between the impurities regardless of their type.

If we allow positions of impurities to move, the distance between impurities would be distributed in the canonical distribution according to the interaction between the impurities in the thermal equilibrium at a given temperature as has demonstrated in the previous paper [17].

V. RESPONCE OF THE LOCAL MAGNETIC STRUCTURE TO THE DYNAMICAL FIELD

In this section we investigate dynamical response of the local magnetic structure (effective $S = 1/2$ spin) induced by a bond impurity to a time-dependent magnetic field with a random noise in the dynamical model (2).

First let us consider the response of the magnetization of a free $S = 1/2$ spin to a sweeping field. The Hamiltonian is given by

$$\mathcal{H}(t) = 2\Gamma S_x - (-H_0 + ct) S_z. \tag{20}$$

This system is two-level system whose energy levels are shown in Fig. 7 as a function of H, where the avoided level crossing occurs near $H = 0$. If $H_0 \gg \Gamma > 0$, the ground state consists primarily of the $M_z = -1/2$ state at $t = 0$. The probability for the system to end up in the $M_z = 1/2$ state (i.e., the probability to change its magnetization) at $t = \infty$ is given by Eq. (10)

Next we consider the case of a local magnetic structure (effective $S = 1/2$) on a lattice. When the noise $\{h_i(t)\}$ does not exist, dynamics of the system is generally the same as that of a free $S = 1/2$ spin as far as we concern the states in an $S = 1/2$ space. It is easily understood as follows. Adopting $\{|+\rangle, |-\rangle\}$ as the basis set, the matrix representation of Eq. (20) is

$$\mathcal{H} = \begin{pmatrix} -\frac{H}{2} & \Gamma \\ \Gamma & \frac{H}{2} \end{pmatrix}. \tag{21}$$

Noting that $\sum_i J_{i,i+1} \mathbf{S}_i \cdot \mathbf{S}_{i+1}$ and $2\Gamma \sum_i S_i^x - H(t) \sum_i S_i^z$ commute, the matrix representation of Eq. (2) in the total $S = 1/2$ space is given by

$$\mathcal{H} = \begin{pmatrix} -\frac{H}{2} + \text{const.} & \Gamma \\ \Gamma & \frac{H}{2} + \text{const.} \end{pmatrix}, \tag{22}$$

adopting $\{|S^{\text{tot}} = 1/2, M_z = 1/2\rangle, |S^{\text{tot}} = 1/2, M_z = -1/2\rangle\}$ as the basis set. The constant in Eq. (22) does not depend on $H(t)$. Thus the dynamics is independent of the number of sites and the combination of $\{J_{ij}\}$.

In the experimental situation, however, noise usually has an influence on the system. If a random noise is applied to each site individually, the term $-\sum_i (H(t) + h_i(t)) S_i^z$ does not commute with $(\mathbf{S}^{\text{tot}})^2 = (\sum \mathbf{S}_i)^2$, and therefore the dynamics would be changed when the interaction $\{J_{ij}\}$ and the system size are varied.

Here for the study of dynamical properties we adopt the minimum model of the type (d) because we can treat a limited number of spins in the scheme of Eq. (3). This model consists of five sites and we take $J_1 = 1.0$ and $J_2 = 0.5$. This is the minimum bond-alternating model with a $J_2 J_2$ bond impurity. This system is looked on as an effective $S = 1/2$ spin.

It would be expected that the effect of noise is reduced as the system size becomes large and a local magnetic structure (effective $S = 1/2$ spin) consisting of several number of spins is less sensitive to such a random noise than a free $S = 1/2$ spin. In order to study effects of the noise we investigate the following properties.

First we study the broadening of the level due to the noise. A energy gap and a sweeping rate at the level crossing point are important factors to determine the transition probability under a sweeping uniform field (see Eq. (10)). It would be useful to investigate how the noise influences the energy gap at the level crossing point. For a single spin the energy gap is given by

$$\Delta E = \sqrt{(2\Gamma)^2 \ + \ (h(t))^2} \tag{23}$$

for $H(t) = 0$. Thus using the distribution of $h(t)$ (a gaussian distribution with the variance $A^2/2\gamma$ in Eq. (8)), we can calculate the mean $\langle \Delta E \rangle$ and the width $\delta E = \sqrt{\langle (\Delta E)^2 \rangle - \langle \Delta E \rangle^2}$, which are listed in Table I. For the local magnetic structure, we calculate the energy gap in a noise by a perturbation method. That gives

$$\Delta E = 2\Gamma + \frac{2|\langle \phi_1^{(0)} | V_1 | \phi_2^{(0)} \rangle|^2}{E_2^{(0)} - E_1^{(0)}} + \text{contributions from higher levels}, \tag{24}$$

where $E_1^{(0)}$ and $\phi_1^{(0)}$ ($E_2^{(0)}$ and $\phi_2^{(0)}$) are the eigenstate of the ground state (the first exited state) of the non perturbed hamiltonian. The term V_1 is $\sum_i h_i S_i^z$. Noting that

$$\langle\ |\langle\phi_1^{(0)}|V_1|\phi_2^{(0)}\rangle|^2\rangle = \sum_i \langle h_i^2\rangle |\langle\phi_1^{(0)}|S_i^z|\phi_2^{(0)}\rangle|^2, \qquad (25)$$

we can calculate $\langle\Delta E\rangle$ from the distribution of $\{h_i\}$, which are also listed in Table I for $L = 5$ and $L = 9$. For large values of A, we obtain the energies by diagonalizing the hamiltonian Eq. (2) and obtained $\langle\Delta E\rangle$ and δE numerically from 500 samples of $\{h_i\}$, which are also listed in Table I. Thus we find the noise causes almost the same effect on the broadening of the energy levels at $H(t) = 0$ in both systems, i.e., a single spin and local magnetic structures, which is not in accordance with the above expectation.

Second, we investigate the dynamical properties of the both systems. In particular, we study the time evolution of magnetization under the sweeping field. We set parameters $\Gamma = 0.02$, $H_0 = 0.5$, $c = 0.0005$, $t_{\max}$=2000, and $dt = 0.01$. In this parameter set the probability p in Eq. (10) is nearly 1. As was mentioned, the responses of the magnetization are the same in both systems when a random noise is not applied. Time evolution without noise is shown by thin dotted lines in Figs. 8 (a)-(c).

Next we investigate the dynamics with the random field (Eq. (6)). We observe the two cases changing the amplitude A of noise (Eq. (7)); (a) $A = 0.01$ and (b) $A = 0.02$. The value of γ is fixed at 0.1. The lowest two energy levels of the system with a random noise $\{h_i(t)\}$ for case (b) are illustrated as a function of time in Fig. 9.

Figure 8 (a) shows $M(t)$ in the noise of a small amplitude ($A = 0.01$). The transition probabilities for a local magnetic structure (effective $S = 1/2$ spin) and an $S = 1/2$ free spin are very close to each other at this small amplitude and the probabilities are reduced by a little amount from the probability of the pure system (i.e., $h_i(t) = 0$). Increasing the amplitude to $A = 0.02$ (Fig. 8 (b)), reduction of $M(t)$s increases. Furthermore we find that $M(t)$ for the local magnetic structure remains larger than that of a free spin. The errorbar shows the first standard deviation of the distribution of $\{M(t)\}$. Here we find that the distribution is rather wide but the mean of the distribution is definitely different. The reduction of $M(t)$ by field fluctuation corresponds to the reduction of p in Eq. (10). The reduction of p has already pointed out for a single spin by Y. Kayanuma and H. Nakayama [29]. Our results are qualitatively consistent with their results. Furthermore, the present observation indicates that a local magnetic structure induced by an impurity is less sensitive to the noise. This feature may be due to this bulky structure of the local magnetic structure. From this observation we may expect that local magnetizations are easier to manipulate than single spins in a field with noise. Detail analysis for the noise dependence will be reported elsewhere.

VI. SUMMARY AND DISCUSSION

In the bond-alternating ($S = 1/2$) Heisenberg antiferromagnetic chain, we studied properties of locally induced magnetic structures by inhomogeneities of the lattice such as the defect of alternation or the edge of the lattice. Because of the gapful nature, the role of the inhomogeneities is similar to that in the Haldane systems and is very different from that in the uniform chain. In the uniform chain we found that the bond impurities divide the system into domains. We showed that a local magnetic structure induced by a bond impurity can be looked on as an effective $S = 1/2$ spin. The interaction between the local magnetic moments decays exponentially in the present model and the local magnetic structures behave almost independently even at very low temperatures.

We also studied the force acting between these defects of alternation. There are several configurations of defects. We investigated the forces between J_1J_1 and J_1J_1, between J_2J_2 and J_2J_2, and between J_1J_1 and J_2J_2. Furthermore, there are two types of separations of defects, i.e., the type of (15) and (17). It turned out that the forces are attractive for all cases.

We also studied the dynamical response of the magnetization to a sweeping field. The induced local moment behaves as a single spin even in dynamical property as far as the uniform field is applied. We considered what property is different between the local magnetic structure (effective $S = 1/2$ spin) induced by an impurity and a free $S = 1/2$ spin. In realistic situation there exists noise which is not necessarily uniform but different from site to site. It has been found that even when noise is applied individually at each site, the total effect of the noise on the broadening of the energy levels is almost the same as that of the single spin. However, the dynamical response of the magnetization to a time-dependent magnetic field with a random noise is found to be different from that of a single spin. That is, the local magnetic structure is found to be more robust against noise applied at each site individually.

The present study is the first attempt treating the dynamics of such a local magnetic structure. We hope that this work provides a basic information for the manipulation of microscopic or nanoscale magnetic devices in the future. We also hope that the present study helps to analyze the magnetic properties at low temperatures such as observed by NMR measurement.

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APPENDIX A: THE CORRELATION LENGTH OF BOND-ALTERNATING CHAIN ($S = 1/2$)

We determined the correlation length of HAF bond-alternating chain ($S = 1/2$) in the ground state as a function of the ratio J_1/J_2. We calculated the correlation function for various ratios (J_1/J_2) and estimated the correlation length using the relation

$$\ln\langle S_i^z S_j^z\rangle = \text{constant} - \frac{r_{ij}}{\xi}, \tag{A1}$$

where r_{ij} denotes the distance between site i and site j, and ξ denotes the correlation length of the system. We treated periodic chains with 60 sites and simulations were performed at $T = 0.01$ in the $M_z = 0$ space. We show the correlation lengths for various ratios (J_1/J_2) in Table II. Here we adopt the length of a pair of bonds J_1 and J_2 to be a unit length, i.e., this unit is double of the bond length.

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FIG. 1. Magnetization profiles $\{m_i\}$ of the models (a)-(d) at $T = 0.01$ in the $M_z = 1/2$ space. (a) and (c) contain 63 sites ($L = 63$) and (b) and (d) contain 65 sites ($L = 65$) . The diamonds denote the strength of bonds $\{J_{i,i+1}\}$, those at high positions denote $J_1 = 1.3$ and those at the low positions denote $J_2 = 0.7$. Details are shown in text.

FIG. 2. Summation of magnetization per site from the left edge site for the model (b).

FIG. 3. Summation of magnetization per site from the left edge site for a bond-alternating chain of the type (b) in Fig. 1 with $L = 21$. The strong and weak bonds are $J_1 = 2$ and $J_2 = 0.5$, respectively.

FIG. 4. Distribution of M_z for the model (b) in Fig. 1.

FIG. 5. Magnetization profile $\{m_i\}$ for a model which has five positions of induced moments in the $M_z = 1/2$ space at $T = 0.01$ with $L = 101$. The diamonds denote the strength of bonds $\{J_{i,i+1}\}$, those at high positions denote $J_1 = 1.3$ and those at the low positions denote $J_2 = 0.7$.

FIG. 6. Ground state energy as a function of (a) Δ_a and (b) Δ_b obtained by an exact diagonalization ($L = 24$, PBC).

FIG. 7. Avoided level crossing.

FIG. 8. Time evolution of magnetization. Thin dotted line denotes the magnetization without noise. Thick line denotes the magnetization of a local magnetic structure (effective $S = 1/2$ spin) of $L = 5$ with a random noise (averaged over 500 samples $\{h_i\}$). Thick dotted line denotes the magnetization of a free $S = 1/2$ spin with a random noise (averaged over 500 samples $\{h_i\}$). (a) $A = 0.01, \gamma = 0.1$, (b) $A = 0.02, \gamma = 0.1$.

FIG. 9. Energy structure of the two level system with a random noise for $A = 0.02, \gamma = 0.1$.

TABLE I. Average energy gaps $\langle \Delta E \rangle$ and their widths δE for several values of $A/\sqrt{2\gamma}$. (1), (5), and (9) mean a single free spin, the minimum model consisting of 5 spins, and the next minimum model consisting of 9 spins of the type (d) in Fig. 1, respectively. The subscript p denotes that the quantities are obtained by the perturbation method and the subscript d denotes that the quantities are obtained by the exact diagonalization method.

TABLE II. Correlation length ξ as a function of the ratio of the J_1/J_2 in the bond-alternating chain ($S = 1/2$)

Table I

$A/\sqrt{2\gamma}$	$\Delta E_{\rm d}(1)$	$\delta E_{\rm d}(1)$	$\Delta E_{\rm p}(5)$	$\Delta E_{\rm d}(5)$	$\delta E_{\rm d}(5)$	$\Delta E_{\rm p}(9)$	$\Delta E_{\rm d}(9)$	$\delta E_{\rm d}(9)$
0.01	0.0412	0.0016	0.0413	0.0412	0.0016	0.0413	0.0413	0.0017
0.02	0.0445	0.0056	0.0450	0.0443	0.0054	0.0450	0.0446	0.0058
0.03	0.0486	0.0105	0.0513	0.0492	0.0111	0.0514	0.0492	0.0112
0.04	0.0542	0.0157	0.0601	0.0544	0.0169	0.0602	0.0546	0.0171
0.05	0.0609	0.0222	0.0714	0.0591	0.0213	0.0716	0.0605	0.0233

Table II

J_1/J_2	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0
ξ	2.02	1.51	1.31	1.18	1.01	0.93	0.84	0.80	0.77